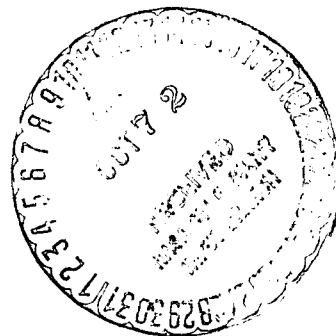


EXCITATION OF ATOMS BY ELECTRON IMPACTS,
AS APPLIED TO THE EXCITATION OF RESONANCE
TRANSITIONS IN THE ISOELECTRONIC SERIES OF
LITHIUM AND SODIUM

O. Bely, J.A. Tully and H. Van Regemorter

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Paris Observatory

(Director: Prof. Andre Danjon)

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EXCITATION OF ATOMS BY ELECTRON IMPACTS,
AS APPLIED TO THE EXCITATION OF RESONANCE TRANSITIONS IN THE ISOELEC-
TRONIC SERIES OF LITHIUM AND SODIUM.

by

Oleg Bely, John Tully and Henri Van Regemorter

Introduction

The first part of the article reports on the methods of computing excitation cross-sections of neutral atoms and of positive ions by electron impact. The article demonstrates that it was necessary to consider both the ion field distribution and the effect of strong coupling in the case of positive ions and optically permissible and intense transitions. The collision ion is represented by Coulomb's waves and the strong couplings are taken into account by applying variation methods in computing the matrix R instead of computing the diffusion S matrix -- as in the Born approximation.

We have applied, in the second part of the article, the theory of the Racah tensor operators to the calculation of potentials intervening in the collision problems. This method permits the computation of ex-

citation cross-sections of atoms and complex ions possessing more than one electron of chemical value. The computations were made for application in a very general case -- for complex transitions -- and may be used in the majority of cases involving possible transitions. We did not calculate the exchange potentials.

The third part of the article deals with the application of the method to the computation of cross-sections in the case of resonance transitions $s - p$ of isoelectric series of lithium and sodium.

All these various approximations are discussed and the results are compared to those obtained by using the method -- excessively work-consuming -- of solving coupled equation problems as well as to those obtained by the easily calculated approximations of Bethe and of the "collision impact parameter". It has been confirmed that the impacts corresponding to the large kinetic moments are predominant with the exception of areas close to the excitation threshold. Consequently, semi-classical approximation may also yield good results as well as the simplified approximation of Bethe -- with the provision that the effect of strong couplings will be taken into account.

1. Method of computing excitation cross-sections

The investigation deals with an atom in the $\alpha L M_L S M_S$ state, where α designates the configuration and the intermediary couplings of the atom $L S M_L M_S$ is the orbital angular momentum, the spin and their projections upon the axis of the Z . The state of the atom will be wholly

characterized by the skew-symmetric amplitude probability $\Psi(\alpha L M_L S M_S | \vec{R})$ where \vec{R} represents the group of coordinates $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N$ of the N atomic electrons ($\vec{r}_i = (r_i, \hat{r}_i, \sigma_i)$).

In a collision problem an electron characterized by its initial velocity rate \vec{v} and by the projection of its spin m_g upon OZ passes close to the atom. Upon the collision the atom is in the $\alpha' L' M_L' S' M_S'$ state and the ultimate state of the collision electron is characterized by \vec{v}' and m_g' .

We will use the following atomic units:

$$(m_e = e = \hbar = 1).$$

Instead of dealing with velocity we will define the impulse $\vec{k} = m_e \vec{v} / \hbar$. k^2 is numerically equal to the kinetic energy of the electron in units of 13.60 e V, and m_e is the mass of the electron.

The amplitude probability represents the primary electron associated with an atomic level and it can decompose into sub-waves corresponding to various orbital angular moments.

$$\varphi(\vec{k}, m_s) = \varphi(\vec{k}) \cdot \delta(m_s | \sigma) = \sum_{lm_l} \varphi(klm_l m_s). \quad (1)$$

The wave function in the overall system -- atom and electron -- will build itself up in accordance with the added kinetic moments properties. If \vec{L} and \vec{S} designate the total angular moment $\vec{L} + \vec{S}$, and the total spin $\vec{S} + \vec{s}$ of the system with $N + 1$ electrons, we will obtain when presenting coupled moments $\Gamma = \alpha L S L' M' S' M_S'$ the following expression:

$$\begin{aligned} \Psi(\Gamma | \vec{R}_{N+1}) = & \sum_{\substack{M_L M_S \\ m_l m_s}} C_{M_L M_S}^{L L' T} C_{m_l m_s}^{S s T} \\ & \times \Psi(\alpha L M_L S M_S | \vec{R}) \cdot \varphi(klm_l m_s | \vec{r}_{N+1}). \end{aligned} \quad (2)$$

This wave function will not be skew-symmetric in relation to the exchange of the $N + 1$ electron with one of the N atomic electrons.

If the exchange is disregarded, the solution of the Schrödinger equation of the system:

$$[H(\vec{R}, \vec{r}_{N+1}) - E]\Psi(\vec{R}, \vec{r}_{N+1}) = 0 \quad (3)$$

could develop along the following:

$$\Psi(\vec{R}, \vec{r}_{N+1}) = \sum_{\Gamma'} \Psi(\Gamma' | \vec{R}, \vec{r}_{N+1} \dots) \quad (4)$$

However, if the exchanges are to be taken into consideration the total overall system should be represented by a linear and skew-symmetric combination of the type:

$$\Psi = \sum_{\Gamma'} \sum_i \frac{(-1)^{N+1-i}}{\sqrt{N+1}} \Psi(\Gamma' | \vec{r}_1, \vec{r}_2 \dots \vec{r}_{i-1}, \vec{r}_{i+1} \dots \vec{r}_{N+1}, \vec{r}_i) \quad (5)$$

where the angular momentum l of the free electron is affected by the electron i .

Radical equations. -- The cross-section is affected by the asymptotic shape of the radial functions of the collision electron. We will, therefore, develop the radial component in

$$\varphi(klm_l m_s | \vec{r}_{N+1}) = \delta(m_s | \sigma_{N+1}) Y_{lm_l}(\hat{r}_{N+1}) \frac{1}{r_{N+1}} F_{kl}(r_{N+1}) \quad (6)$$

where the $Y_{lm_l}(\hat{r})$ are the normalized spherical harmonics, such as:

$$\int Y_{l'm'}(\hat{r}) Y_{lm}(\hat{r}) d\hat{r} = \delta_{ll'} \delta_{mm'} \quad (7)$$

with $\hat{r} = \frac{\vec{r}}{|\vec{r}|}$ et $d\hat{r} = \sin \theta d\theta d\varphi$.

It is expedient to introduce the function, as suggested by Percival and Seaton (13) in the coupled development Γ

$$\Psi(\Gamma | \vec{R} \hat{r}_{N+1} \sigma_{N+1}) = \sum_{M_L M_S m_l m_s} C_{MM^T}^{LL^T} C_{M_S m_s M_S^T}^{S_S^T} \times \Psi(\alpha LSM_L M_S | \vec{R}) \delta[m_s | \sigma_{N+1}] Y_{lm_l}(\hat{r}_{N+1}) \quad (8)$$

function of all the variables with the exception of the radial variable r_{n+1} .

In this development the wave functions of the overall system will be as follows:

$$\Psi(\Gamma' | \vec{R}_{r_{N+1}}) = \sum_{\Gamma} \Psi(\Gamma | \vec{R}_{r_{N+1}} \sigma_{N+1}) \frac{1}{r_{N+1}} F_{\Gamma}(\Gamma' | r_{N+1}). \quad (9)$$

The asymptotic shape of this wave function contains a plane wave associated with the initial atom and with diffused waves associated with all other atoms. Here Γ' is the initial state of the system.

In order to determine the radial equations which must satisfy the $F_{\Gamma}(\Gamma' | r_{N+1})$ we shall isolate the radial components by effecting the scalar product

$$\int \Psi^*(\Gamma | \vec{R}_{r_{N+1}} \sigma_{N+1}) [H - E] \Psi(\Gamma' | \vec{R}_{r_{N+1}}) d\vec{R} d\vec{r}_{N+1} d\sigma_{N+1} \quad (10)$$

integrating in the entire space $\hat{R}, \hat{r}_{N+1}, \sigma_{N+1}$.

The total hamiltonian will be presented as:

$$H[\vec{R}, \vec{r}_{N+1}] = H_1(R) + H_2(\vec{r}_{N+1}) + \sum_{i=1}^N \frac{1}{r_{N+1,i}}. \quad (11)$$

$H_1(R)$ is the atom hamiltonian and affects only atomic wave functions.

$$H_2(\vec{r}_{N+1}) = -\frac{1}{2} \Delta_{N+1} - \frac{Z}{r_{N+1}}$$

is the free electron hamiltonian in the nucleus field. Z is the charge of the nucleus.

$r_{N+1,i}$ is the distance between the collision electron and the atomic electron i .

On the other hand, the total energy of the system is preserved:

$$E = E_a + \frac{1}{2} k_a^2 = E_a' + \frac{1}{2} k_a'^2 \quad (12)$$

where α shows the state of the atom $\alpha L S M_L M_S$.

Radial equations are obtained:

$$\left[\frac{d^2}{dr_{N+1}^2} - \frac{l(l+1)}{r_{N+1}^2} + \frac{2Z}{r_{N+1}} + k_a^2 \right] F_{\Gamma}(\Gamma' | r_{N+1}) = 2 \sum_{\Gamma''} V_{\Gamma \Gamma''} F_{\Gamma''}(\Gamma' | r_{N+1}) \quad (13)$$

with

$$V_{\Gamma \Gamma'}(\Gamma_{N+1}) = \int \Psi_{\Gamma'}^*(\vec{R} \hat{r}_{N+1} \sigma_{N+1}) \sum_{i=1}^N \frac{1}{r_{N+1,i}} \Psi_{\Gamma}(\vec{R} \hat{r}_{N+1} \sigma_{N+1}) d\vec{R} d\hat{r}_{N+1} d\sigma_{N+1}. \quad (14)$$

Thus, we have to solve a system of coupled differential equations.

In the collision problem if the total angular momentum and the total spin are preserved and we obtain $L^T = L^{T'}$, $S^T = S^{T'}$, $M_L^T = M_L^{T'}$, $M_S^T = M_S^{T'}$.

In addition, the $V_{\Gamma \Gamma'}$ potentials in the LS coupling are independent of S^T and independent in the choice of axes, thereby of M_S^T , M_L^T . The radial functions will therefore depend only upon the parameters of $\alpha L S / L^T$.

In order to solve this type of equations system, even with the aid of computers it will be necessary to make various approximations. In addition to limiting the number of the $\alpha L S$ levels of the atom we will have to disregard the continuous states implied in principle in the summation of equation (9). If only two levels are investigated, for instance, the $\alpha L S$ initial level and the $\alpha' L' S'$ final one all the processes:

$$\alpha L S \rightarrow \alpha'' L'' S'' \rightarrow \alpha' L' S'$$

will be neglected, which could disturb the $\alpha L S \rightarrow \alpha' L' S'$ process. Coupling between various states of the system is a direct result of the coupling

between the preceding equations.

In accordance with the principle of conservation of parity we must have: $(-1)^{l+l'} = (-1)^{l'+l'}$. (15)

Born and Coulomb-Born Approximations

We start by disregarding any coupling between the states of the system. We call Γ the initial state and Γ' the final state. The total wave functions will then be reduced to:

$$\Psi(\Gamma | \vec{R}_{r_{N+1}}) = \Psi(\Gamma | \vec{R}_{r_{N+1}} \sigma_{N+1}) \frac{1}{r_{N+1}} F_{\Gamma}(\Gamma | r_{N+1}). \quad (16)$$

The radial equations will be reduced to two uncoupled equations:

$$\begin{aligned} \left[\frac{d^2}{dr_{N+1}^2} - \frac{l(l+1)}{r_{N+1}^2} + \frac{2Z}{r_{N+1}} + k_a^2 \right] F_{\Gamma}(\Gamma | r_{N+1}) &= 2V_{\Gamma\Gamma} F_{\Gamma}(\Gamma | r_{N+1}) \\ \left[\frac{d^2}{dr_{N+1}^2} - \frac{l'(l'+1)}{r_{N+1}^2} + \frac{2Z}{r_{N+1}} + k_{a'}^2 \right] F_{\Gamma'}(\Gamma' | r_{N+1}) &= 2V_{\Gamma'\Gamma'} F_{\Gamma'}(\Gamma' | r_{N+1}). \end{aligned} \quad (17)$$

In the Born approximation only the asymptotic form of the potentials $V_{\Gamma\Gamma}$ is taken into consideration. For $r_{N+1} \gg r_0$ we have $r_{N+1,i} = r_{N+1}$ and $V_{\Gamma\Gamma} = \frac{N}{r_{N+1}}$.

In this manner two equations of the type:

$$\left[\frac{d^2}{dr_{N+1}^2} - \frac{l(l+1)}{r_{N+1}^2} + \frac{2(Z-N)}{r_{N+1}} + k^2 \right] F_{kl}(r_{N+1}) = 0 \quad (18)$$

are found, where the radial function depends only upon k , l and $Z - N = z$.

In case of a neutral atom $z = 0$, the two conditions for limits are:

$$F_{kl}^n(0) = 0 \quad F_{kl}^n(r \rightarrow \infty) \rightarrow k^{-1/2} \sin \left[kr - \frac{l\pi}{2} \right] \quad (19)$$

we obtain, in fact:

$$F_{kl}^n(r) = k^{-1/2} j_l(kr) \quad (19')$$

with

$$j_l(kr) = \left[\frac{\pi kr}{2} \right]^{1/2} J_{l+1/2}(kr)$$

where $J_{l+1/2}$ is the Bessel spherical function.

In the case of an ionized atom the same approximation will be designated as the "Coulomb-Born approximation" to precisely point out the fact that the Coulomb potential has been taken into account in z/r_{N+1} while determining the radial function.

The two limit conditions are:

$$\begin{aligned} \Gamma_{kl}^{CB}(0) = 0 \quad \Gamma_{kl}^{CB}(r \rightarrow \infty) &\rightarrow k^{-1/2} \sin \left[kr - \frac{l\pi}{2} \right] \\ &+ \frac{z}{k} \log(2kr) + \arg \Gamma \left(l + 1 - \frac{iz}{k} \right). \end{aligned} \quad (20)$$

It can be proven that:

$$\begin{aligned} \Gamma_{kl}^{CB}(r) = \frac{2^l}{(2l+1)!} e^{\frac{\pi z}{2k}} \Gamma \left(l + 1 - i \frac{z}{k} \right) k^{-1/2} e^{ikr} (kr)^{l+1} \\ F \left[l + 1 - i \frac{z}{k}, 2l+2, -2ikr \right] \end{aligned} \quad (21)$$

where $F(a, b, t)$ is the confluent hypergeometric function.

In the Born approximation -- as can be now observed -- the functions of an approximated wave of the collision electron are plane waves both after and prior to the collision. When they are computed no consideration is given to the disturbance due to waves diffused by all possible states of the system.

In general, solutions of coupled equations do not have the asymptotic forms (19) and (20).

If we would like to present the system in the state Γ we would

have to know all the functions $F_{\Gamma''}(\Gamma | r)$ -- each a function of one of the states Γ'' possible in the system.

Each radial function will have an asymptotic form (16):

$$F_{\Gamma''}(\Gamma | r) \xrightarrow{r \rightarrow \infty} k_{\Gamma''}^{-1/2} \left[\delta_{\Gamma\Gamma''} \sin \left(k''r - \frac{l''\pi}{2} \right) + R_{\Gamma\Gamma''} \cos \left(k''r - \frac{l''\pi}{2} \right) \right] \quad (22)$$

for the neutral atoms. For positive ions it is sufficient to substitute the sine and cosine functions by:

$$k''r - \frac{l''\pi}{2} + \frac{z}{k''} \log(2k''r) + \arg \Gamma \left(l + 1 - \frac{iz}{k''} \right).$$

When the coupling is disregarded ($\Gamma'' = \Gamma$) the forms are easily detected (19) and (20). The terms of the matrix R called the reactance matrix,

$R_{\Gamma\Gamma''}$ show amplitudes of diffused waves which correspond to all possible states of the system.

Upon a numerical resolution of the differential equation system (13) it is possible to conceive the definition of the terms of the R matrix starting from the asymptotic forms of solutions.

Variational Method Applied to the Computation of R

In order to compute the terms of the matrix R it should be possible to solve, in a precise manner, the equation of the system:

$$[H(\vec{R}, \vec{r}) - E]\Psi(\vec{R}, \vec{r}) = 0. \quad (23)$$

We have disregarded the exchange and we have seen that in order to solve the system of coupled equations we should limit ourselves to a small number of states. In the Born and Coulomb-Born approximations, we have substituted in the total hamiltonian H and the terms of electro-

static interaction $\sum_{i=1}^N \frac{1}{r_{N+1,i}}$ by their asymptotic expression $\frac{N}{r_{N+1}}$.

Instead of:

$$H(\vec{R}, \vec{r}) = H_1(\vec{R}) - \frac{1}{2} \nabla_{N+1}^2 - \frac{Z}{r_{N+1}} + \sum_{i=1}^N \frac{1}{r_{N+1,i}} \quad (24)$$

we have, in this last case, used the approximated hamiltonian H' as:

$$H - H' = \sum_{i=1}^N \frac{1}{r_{N+1,i}} - \frac{N}{r_{N+1}}. \quad (25)$$

H' is, then, an approximated hamiltonian. We can solve the equation: $[H' - E] \tilde{\Psi}_R(\vec{R}, \vec{r}) = 0$

whose precise solutions are approximate functions $\tilde{\Psi}$.

By generalization of the variational method of Hulthen and Kohn (12) applied to an inelastic case it is possible to find the precise expression for terms of the matrix R in relation to approximate expressions and errors $\delta\Psi$ related to the wave functions.

$$R_{RR'}(\text{exact}) = R_{RR'}(\text{approx.}) - 2L_{RR'} - 2 \int \delta\Psi_R [H - E] \delta\Psi_{R'} d\vec{r} d\vec{R} \quad (26)$$

with:

$$L_{RR'} = \int \tilde{\Psi}_R [H - H'] \tilde{\Psi}_{R'} d\vec{r} d\vec{R} \quad (27)$$

where H is the exact hamiltonian.

A very satisfying evaluation of the R terms can be arrived at by disregarding in the $R_{RR'}(\text{exact})$ expression the square-law terms in relation to $\delta\Psi$ errors.

In the approximations of Born (B) and Coulomb-Born (C.B.) we have seen that all the couplings were disregarded and that asymptotic forms of radial functions $F_{\Gamma'}(\vec{r})$ were presented by (19) and (20) for $\Gamma = \Gamma'$. For $\Gamma \neq \Gamma'$, however, there is: $F_{\Gamma'}(\vec{r}) = 0$.

Consequently, the terms $R_{RR'}(\text{approximate})$ are zero and we obtain sim-

ply: $R_{\Gamma\Gamma'}^{\text{Born}} = -2 \int \tilde{\Psi}_{\Gamma}^* (\text{Born}) |H - H'| \tilde{\Psi}_{\Gamma'} (\text{Born}) d\vec{r} d\vec{R}$ (28)

with $H - H'$ given by the equation (25).

This last expression should be correlated with that of the potentials $V_{\Gamma\Gamma'}$. We find that:

$$V_{\Gamma\Gamma'} (\text{Born ou COULOMB-Born}) = -2 \int_0^\infty F_{kl}(r_{N+1}) \left[V_{\Gamma\Gamma'} - \delta_{\Gamma\Gamma'} \frac{N}{r_{N+1}} \right] F_{k'l'}(r_{N+1}) dr_{N+1}. \quad (29)$$

The radial functions $F_{kl}(r_{N+1})$ for positive ions (C.B. approximation) are given by equation (21). Satisfactory results may also be obtained for terms of the R matrix by using solely the approximate wave functions: plane waves in the case of neutral atoms, Coulomb waves in the case of positive ions.

Expressions for the Collision Cross-section

We would like to compute the collision excitation cross-section of an atom passing from the state $\alpha L S$ into the state $\alpha' L' S'$.

In presenting $\gamma = \alpha L M_L S M_S l m_l m_s$ after summation for all the final states and the average for all the initial states $(2L + 1)(2S + 1)$ times decomposed and on incident spins we have:

$$\begin{aligned} & \alpha L S \rightarrow \alpha' L' S' \\ & = \frac{1}{2k_a^2} \frac{1}{\omega_{\alpha L S}} \sum_{\substack{M_L M_L' M_S M_S' \\ m_l m_l' m_s m_s'}} |T_{\gamma\gamma'}|^2 \quad \text{in units of } \pi a_0^2 \quad (30) \end{aligned}$$

$\omega_{\alpha L S} = (2L + 1)(2S + 1)$ is the statistical weight of the initial $\alpha L S$ level.

The preceding expression allows the computation of any cross-section of neutral atoms and any inelastic cross-section of positive ions. The matrix T is expressed simply in terms of the diffusion ma-

trix S and this in terms of the R matrix (15).

Inasmuch as the total angular momentum $L^T M^T$ and the total spin $S^T M^T$ are preserved separately, there is an advantage in using the coupled expression $\Gamma = \alpha LS/L^T S^T M_L^T M_S^T$, in which each wave function will have the form:

$$\Psi_{\Gamma}(\vec{R}, \vec{r}) = \sum_{\gamma} (\gamma | \Gamma) \Psi_{\gamma}(\vec{R}, \vec{r}). \quad (31)$$

The unitary matrices of transformation are expressed in terms of Clebsch-Gordan coefficients:

$$\langle \gamma' | \Gamma \rangle = (\Gamma | \gamma') = \delta[\alpha' S' L' I', \alpha S L I] C_{M_L M_L^T M_S M_S^T}^{L L^T} C_{M_S M_S^T}^{S S^T}. \quad (32)$$

The matrix T is transformed following:

$$T_{\gamma\gamma'} = \sum_{\Gamma\Gamma'} (\gamma | \Gamma) T_{\Gamma\Gamma'} (\Gamma' | \gamma'). \quad (33)$$

The collision cross-section is independent of:

$$Q[\alpha LS \rightarrow \alpha' L' S'] = \frac{1}{2k_a^2} \frac{1}{2S+1} \frac{1}{2L+1} \sum_{M_L^T M_S^T} |T_{\Gamma\Gamma'}|^2. \quad (34)$$

The Γ expression represents the matrix T at this point as being diagonal in L^T and M^T , in S^T and M^T . The system being invariant due to rotation, T is independent from M_L^T and M_S^T . In coupling $L - S$, T will not depend upon the total spin S^T . There the $2L^T + 1$ values of M_S^T corresponding to S^T .

$$Q[\alpha LS \rightarrow \alpha' L' S'] = \frac{1}{2k_a^2} \frac{1}{2S+1} \frac{1}{2L+1} \sum_{M_L^T M_S^T} (2L^T+1)(2S^T+1) |T_{\alpha LS, \alpha' L' S'}|^2. \quad (35)$$

In the coupled expression, the summation is reduced to the summation of the three variables $11 L^T$. L^T may possess all the values:

$$|L-l|, |L-l+1|, \dots, |L+l|.$$

The T matrix and the R matrix are connected by means of the exact relation (15): $T = -\frac{2iR}{1-iR}$. (36)

The R matrix is real and symmetric. It is easy to demonstrate that the T matrix is symmetric and that the scattering matrix $I - T = S$ is unitary.

$$S = \frac{I + iR}{I - iR} \quad (37)$$

from where $S + S^\dagger = 1 = SS^\dagger$ ($A^\dagger =$ an associated transposition).

Physically, this means that the scattered (diffused) flux equals the incident flux. On the other hand, due to the fact that T is symmetric, the probability of the alphaLS state being excited to the alpha'L'S' state equals the probability of the inverse (reciprocal) process:

$$\begin{aligned} (2S + 1)(2L + 1)k_a^2 Q[\alpha LS \rightarrow \alpha' L' S'] \\ = (2S' + 1)(2L' + 1)k_a^2 Q[\alpha' L' S' \rightarrow \alpha LS]. \end{aligned} \quad (38)$$

By computing the R matrix by an approximate and variational method and then the T matrix by means of equation (36) we have certainly verified the principle of flux conservation, in other words we have a unitary scattering matrix. Seaton (15) has demonstrated that much better results were obtained in this manner than by applying the variational method directly to the computation of S.

This last method applied to the Born approximation would have resulted in:

$$T = 2iR \text{ (Born)} \quad (39)$$

which is identical to (36) only for all $R_{rr} \ll 1$, thus $T \ll 1$.

We will designate the results obtained from the preceding equation as Born I, and those obtained from the exact equation below as Born II:

$$T \text{ (Born II)} = - \frac{2iR \text{ (Born I)}}{1 - iR \text{ (Born I)}}. \quad (40)$$

An analogous formula would be obtained in the case of positive ions (CBII and CBI).

We see that in this manner the effects of coupling have been taken into account in an indirect fashion and only to a certain extent. If, in the Born and the Coulomb-Born approximations they have been disregarded in favor of calculation of the wave functions and of the radial functions, the formula (40) shows that the computation of each term of Γ is affected by all the R terms which cannot be disregarded. We can state that the method II considers all effects of strong couplings.

Born and Coulomb-Born Approximation.

Calculating Terms of the R Matrix

The R matrix terms are given by the equation (29), where, for reasons already explained we may replace Γ by $\alpha LS/L^*$.

In the following chapter we will deal with the computations of the $V_{\Gamma\Gamma'}$ potentials in the general case of complex atoms. Keeping in mind the application to the elements of isoelectric series of Na and Li, we shall start by the simple case of positive atoms or ions possessing only one electron outside of the closed shells.

$$V_{\Gamma\Gamma'} = \int \Psi^*(\Gamma | \vec{r}_1 \hat{r}_2 \sigma_2) \frac{1}{r_{12}} \Psi(\Gamma' | \vec{r}_1 \hat{r}_2 \sigma_2) d\vec{r}_1 d\hat{r}_2 d\sigma_2. \quad (41)$$

We will use the multipolar development of r_{12}^{-1} in the Legendre polynome series:

$$\frac{1}{r_{12}} = \sum_{\lambda} P_{\lambda}(\hat{r}_1 \cdot \hat{r}_2) \gamma_{\lambda}(r_1, r_2) \quad (42)$$

with

$$\gamma_{\lambda}(r_1, r_2) = \begin{cases} r_1^{\lambda}/r_2^{\lambda+1} & \text{for } r_2 > r_1 \\ r_2^{\lambda}/r_1^{\lambda+1} & \text{for } r_1 > r_2. \end{cases} \quad (43)$$

Based on the theorem of addition of spherical harmonics:

$$P_{\lambda}(\hat{r}_1, \hat{r}_2) = \frac{4\pi}{2\lambda + 1} \sum_{\mu} Y_{\lambda\mu}(\hat{r}_1) Y_{\lambda\mu}^*(\hat{r}_2). \quad (44)$$

It is thus possible to develop the integral (41) in terms of λ and to separate the radial integral from the angular summation.

We will always have $S = S' = \frac{1}{2}$ in atoms with one electron valence, the configuration will be determined exactly by the main quantum number n . Thus, in the coupled presentation we will have for $\beta \neq \beta'$:

$$R[\underbrace{nLL}_{\beta}, \underbrace{n'L'L'}_{\beta'}] = -2 \left(nLL \left| \frac{1}{r_{12}} \right| n'L'L' \right) \quad (45)$$

We can state that the only contributions (see II) which are not zeroes are those for which:

$$\begin{aligned} |L - L'| &\leq \lambda \leq L + L' \\ |l - l'| &\leq \lambda \leq l + l' \end{aligned} \quad (46)$$

$L + L' + \lambda$ et $l + l' + \lambda$ are even numbers.

It is easy, by using the multipolar development of r_{12}^{-1} and the wave functions (31) to demonstrate that $R_{\beta\beta'}$ can be presented as:

$$R_{\beta\beta'} = -2 \sum_{\lambda} f_{\lambda}(LL'L'L') \mathcal{R}_{\lambda} \quad (47)$$

with:

$$f_{\lambda} = \frac{4\pi}{2\lambda + 1} \sum_{mm'm'\mu} C_{m_L m_L' m_L}^{LL'L'} C_{m_M' m_M' m_L}^{L'L'L'} \int Y_{LM}^* Y_{\lambda\mu} Y_{L'M'} d\hat{r}_1 \times \int Y_{lm}^* Y_{\lambda\mu} Y_{l'm'} d\hat{r}_2 \quad (48)$$

and:

$$\mathcal{R}_{\lambda} = \int_0^{\infty} F_{kl}(r_2) F_{k'l'}(r_2) \int_0^{\infty} \gamma_{\lambda}(r_2) P_{nL}(r_1) P_{n'L'}(r_1) dr_1 dr_2 \quad (49)$$

where the functions $P_{nL}(r)$ are the radial functions of the wave functions of the optical electron:

$$\Psi(nLM_L | \vec{r}_1) = Y_{LM}(\hat{r}_1) \frac{1}{r_1} P_{nL}(r_1). \quad (50)$$

By disregarding the spins in (8) we obtain, in fact:

$$\Psi(\vec{r}_1 \vec{r}_2) = \sum_{m_L m_l} C_{m_L m_l}^{L L' T} \Psi(n L M | \vec{r}_1) Y_{l m}(\vec{r}_2). \quad (51)$$

By using the composition equation of spherical harmonics:

$$\begin{aligned} & \int Y_{L M}^*(\vec{r}) Y_{\lambda \mu}(\vec{r}) Y_{L' M'}(\vec{r}) d\vec{r} \\ &= \frac{1}{\sqrt{4\pi}} \left[\frac{(2\lambda + 1)(2L' + 1)}{2L + 1} \right]^{1/2} C_{M' \mu M}^{L \lambda L} C_{000}^{L' \lambda L} \quad (52) \end{aligned}$$

as well as the relations between the Racah coefficients W and the Wigner coefficients $3j$ we arrive at a result which will be determined below by the method of tensor operators of Racah (9) and (14):

$$\begin{aligned} f_{\lambda} &= \langle L L' M_L^T | P_{\lambda}(\vec{r}_1, \vec{r}_2) | L' L' M_L^T \rangle \\ &= (2\lambda + 1)^{-1} (-1)^{L+L'-L^T} \quad (53) \\ &\times \left[(2L + 1)(2L' + 1)(2L + 1)(2L' + 1) \right]^{1/2} \\ &\quad C_{000}^{L \lambda} C_{000}^{L' \lambda} W(L L' L', L^T \lambda). \end{aligned}$$

The $f_{\lambda}(L L' L' L^T \lambda)$ coefficients have been tabulated by Percival and Seaton (13).

In the radial term \mathcal{R} , the radial functions $F_{kl}(r_2)$ are given by (19') for the neutral ions and in (21) for the positive ions. We shall use the most suitable ones at our disposal when working with radial atomic functions $P_{nL}(r_1)$.

Let us take:

$$Y_{\lambda} = \int_0^{\infty} \gamma_{\lambda}(r_1 r_2) P_{nL}(r_1) P_{n'L'}(r_1) dr_1.$$

In accordance with (43) we can write:

$$\begin{aligned} Y_{\lambda}(r_1) &= \frac{1}{r_2^{\lambda+1}} \int_0^{r_1} P_{nL}(r_1) P_{n'L'}(r_1) r_1^{\lambda} dr_1 \\ &+ r_2^{\lambda} \int_{r_1}^{\infty} P_{nL}(r_1) P_{n'L'}(r_1) \frac{1}{r_1^{\lambda+1}} dr_1. \quad (54) \end{aligned}$$

It is expedient to decompose Y_{λ} into two parts, one representing

the long-range action $[r_2 > r_1]$, and the other which converges rapidly:

$$V_{\lambda}(r_1) = \frac{1}{r_2^{\lambda+1}} \int_0^{\infty} P_{nL} P_{n'L'} r_{\lambda} dr_1 + Z_{\lambda}[nL, n'L' | r_2] \quad (55)$$

with

$$Z_{\lambda} = r_2^{\lambda} \int_{r_1}^{\infty} P_{nL} P_{n'L'} \frac{1}{r_1^{\lambda+1}} dr_1 - \frac{1}{r_2^{\lambda+1}} \int_{r_2}^{\infty} P_{nL} P_{n'L'} r_1^{\lambda} dr_1. \quad (56)$$

Thus, the R_{λ} may be expressed as the sum of two integrals; the first can be calculated by the analytical method; the second, which depends upon the atom properties, converges rapidly:

$$S_{\lambda} = \int_0^{\infty} P_{nL}(r_1) P_{n'L'}(r_1) r_1^{\lambda} dr_1 \int_0^{\infty} F_{kL} F_{k'L'} \frac{dr_2}{r_2^{\lambda+1}} + \int_0^{\infty} Z_{\lambda}(nL, n'L' | r_2) F_{kL} F_{k'L'} dr_2. \quad (57)$$

In the case of neutral atoms the integrals:

$$\int FF' \frac{dr}{r^{\lambda+1}}$$

are reduced to integrals:

$$\int_0^{\infty} J_{l+\frac{1}{2}}(kr) J_{l'+\frac{1}{2}}(kr) r^{-\lambda} dr.$$

In the case of positive ions, the Coulomb integral:

$$I_{\lambda} = \int FF' r^{-\lambda-1} dr$$

converges very slowly for $\lambda = 0$ and $\lambda = 1$. It is possible to find for them analytical expressions (20).

We recognize in R_{λ} the integral $\int_0^{\infty} PP' r^{\lambda} dr$ which intervenes in the calculation on the probability of radiative transition $S_{\lambda}(nL, n'L')$.

We have, for a dipolar transition:

$$S_1(nL, n'L') = 2L > \left| \int_0^{\infty} P_{nL} P_{n'L'} r dr \right|^2 \quad (58)$$

where $L >$ is the largest number (comparing L and L').

Having computed in this manner the terms of the R matrix we obtain T by means of (36) and the component $Q(nL \rightarrow n'L')$ by using equation (34).

Upon summation with S^T we obtain:

$$Q[nL \rightarrow n'L'] = \frac{1}{k_{nL}^2} \frac{1}{2L+1} \sum_{n'L'} (2L'+1) |T_{nL, L', n'L', L'}|^2. \quad (59)$$

In order to reveal the contributions of various kinetic moments we will sum up with the l and l' .

If we express the collision cross-section as a probability function $\Omega(i, j)$:

$$Q(i \rightarrow j) = \frac{1}{\omega_i} \frac{1}{k_i^2} \Omega(i, j) \text{ in units of } \pi a_0^2 \quad (60)$$

$$\Omega[nL, n'L'] = \sum_{L''} \Omega^{L''} \quad \text{with} \quad (61)$$

$$\Omega^{L''} = \sum_{ll'} (2L'' + 1) |T_{nlL'', n'L'L''}|^2.$$

II. Generalization in Cases of Complex Atoms

In cases of atoms possessing more than one outer electron outside of closed shells, the $V_{rr'}$ potentials and the terms of the R matrix are computed by applying the tensor operators theory of Racah.

It is clear from the very expression of these potentials that there is little difference between computations used for them and the computation of the matrix elements in terms of Coulomb interaction of the atom hamiltonian, elements which intervene in the calculation of energy levels when the configuration interaction is particularly taken into consideration. It is well known that the Racah methods for complex atoms are very efficient for such cases (9) and (14). As far as we are concerned we shall apply ourselves to the computation of the $V_{rr'}$ potentials, disregarding in the present article the exchange potentials and by considering the case of the LS coupling.

If, for example, we study the excitation of the Fe XIV(4) we will

find allowed transitions of the $3s^2 3p \rightarrow 3s 3p^2$ type corresponding to the excitation of an electron in an inner shell.

Similarly, all transitions between the fundamental level and the first excited levels of such elements as Be, B, C, N, -- transitions which correspond to the important ultra-violet rays, are of the $2s^2 2p^n \rightarrow 2s 2p^{n+1}$ type.

Consequently, we shall give a privileged treatment to the computations of transitions of the type:

$$l^{n-p}p \rightarrow l^{n-p-1}p+1$$

and present the results for other types of transitions below.

The results are presented under a very general aspect as functions of algebraic coefficients, particularly the W of Racah, the X of Wigner and the fractional parentage coefficients (see appendix C. Messiah, Quantum Mechanics, for tables). The calculations here are presented for the purpose of future use in the computations of cross-sections for elements of the series Be, B, C and N.

Expression of Potentials. -- Let us return to the expression (41) of the

$V_{\Gamma\Gamma'}$:

$$V_{\Gamma\Gamma'}(r_{N+1}) = \int \Psi_{\Gamma'}^*(\vec{R}, \hat{r}_{N+1}, \sigma_{N+1}) \left[\sum_{i=1}^N \frac{1}{r_{n+1,i}} \right] \Psi_{\Gamma}(\vec{R}, \hat{r}_{N+1}, \sigma_{N+1}) d\vec{R} d\hat{r}_{N+1} d\sigma_{N+1} \quad (\Gamma' \neq \Gamma) \quad (41)$$

where the functions Ψ are skew-symmetric only in relation to electrons 1, 2, ..., N. In this presentation, the collision electron is characterized by its kinetic moment (l_1'' before the collision, l_1'' after the collision) and the spin of $\frac{1}{2}$. Thus, we can still write $V_{\Gamma\Gamma'}$ under the

more symbolic form:

$$V_{\Gamma\Gamma'}(r_{N+1}) = (\alpha L S l_1 \frac{1}{2} L^r M_L^r S^r M_s^r \left| \sum_{i=1}^N \frac{1}{r_{N+1,i}} \right| \alpha' L' S' l_1' \frac{1}{2} L^r M_L^r S^r M_s^r) \quad (62)$$

where it is understood that the scalar product does not affect r_{N+1} .

Instead of representing the total system by quantum numbers $\alpha L S l_1 \frac{1}{2} L^r M_L^r S^r M_s^r$,

we may also present it by an assembly of quantum numbers as follows:

$\alpha L S m_s l_1 \frac{1}{2} m_s L^r M_L^r$. In fact, all the operators associated to these quantum numbers inter-commute and, consequently, this assembly of quantum numbers is an assembly equivalent to the precedent. We may, then, write $V_{\Gamma\Gamma'}$ in the following manner:

$$V_{\Gamma\Gamma'}(r_{N+1}) = \sum_{\substack{M_s M_s' \\ m_s m_s'}} \langle S \frac{1}{2} S^r M_s^r | S \frac{1}{2} M_s m_s \rangle \langle S' \frac{1}{2} M_s' m_s' | S' \frac{1}{2} S^r M_s^r \rangle \cdot (\alpha L S m_s l_1 \frac{1}{2} m_s L^r M_L^r \left| \sum_{i=1}^N \frac{1}{r_{N+1,i}} \right| \alpha' L' S' M_s' l_1' \frac{1}{2} m_s' L^r M_L^r) \quad (63)$$

Inasmuch as $\sum_{i=1}^N \frac{1}{r_{N+1,i}}$ does not depend upon spins, we have:

$$M_s = M_s' \quad S = S' \quad \text{and} \quad m_s = m_s'$$

The summation becomes:

$$V_{\Gamma\Gamma'}(r_{N+1}) = \sum_{M_s m_s} \langle S \frac{1}{2} S^r M_s^r | S \frac{1}{2} M_s m_s \rangle \langle S \frac{1}{2} M_s m_s | S \frac{1}{2} S^r M_s^r \rangle \cdot (\alpha L S m_s l_1 \frac{1}{2} m_s L^r M_L^r \left| \sum_{i=1}^N \frac{1}{r_{N+1,i}} \right| \alpha' L' S M_s l_1' \frac{1}{2} m_s L^r M_L^r) \quad (64)$$

The $\langle J_1 J_2 J M | j_1 j_2 m_1 m_2 \rangle$ are the Clebsch-Gordan coefficients expressed otherwise as: $C_{m_1 m_2 M N}^{J_1 J_2 J}$.

We will now transform:

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}}$$

As in (42)

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}} = \sum_{i=1}^N \left(\sum_{\lambda=0}^{\infty} \gamma_{\lambda}(r_{N+1,i}) P_{\lambda}(\widehat{r}_i, \widehat{r}_{N+1}) \right) \quad (65)$$

$P_{\lambda}(x)$ is the polynome of Legendre of the λ order;

$$\gamma_{\lambda}(r_{N+1,i}) = \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}}$$

where $r_{<}$ is the smallest of the lengths r_{N+1} and r_i and $r_{>}$ the largest of the lengths r_{N+1} and r_i .

Using the theorem of addition of spherical harmonics we may put this in the following form:

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}} = \sum_{i=1}^N \left(\sum_{\mu\lambda} \frac{4\pi}{2\lambda+1} \gamma_{\lambda}(r_{N+1,i}) Y_{\lambda\mu}^*(\widehat{r}_{N+1}) Y_{\lambda\mu}(\widehat{r}_i) \right) \quad (66)$$

fully utilizing the fact that

$$Y_{\lambda\mu}^*(\widehat{r}) = (-)^{\mu} Y_{\lambda-\mu}(\widehat{r})$$

and presenting:

$$C_{\mu}^{(\lambda)}(\widehat{r}) = \left(\frac{4\pi}{2\lambda+1} \right)^{1/2} Y_{\lambda\mu}(\widehat{r})$$

we see that:

$$\sum_i \frac{1}{r_{N+1,i}}$$

may be presented in the following form:

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}} = \sum_{\lambda} \left\{ \sum_{\mu} (-)^{\mu} \left(\sum_{i=1}^N \gamma_{\lambda}(r_{N+1,i}) C_{\mu}^{(\lambda)}(i) \right) C_{-\mu}^{(\lambda)}(\widehat{r}_{N+1}) \right\} \quad (67)$$

Now, this appears as a sum on λ of scalar products of tensor operators, the first acting on the angular variables of the ^{atom} the second, on the angular variables of the incident electron. Setting it more precisely the tensor operator acting upon the atom is:

$$T_{\mu}^{(\lambda)} = \sum_{i=1}^N U_{\mu}^{(\lambda)}(\widehat{i}, i, r_{N+1}) = \sum_{i=1}^N \gamma_{\lambda}(r_{N+1}, r_i) C_{\mu}^{(\lambda)}(\widehat{i}) \quad (68)$$

while that which acts upon the incident electron is: $C_{-\mu}^{(\lambda)}(\hat{r}_{N+1})$.

In this manner

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}}$$

is presented in the form:

$$\sum_{i=1}^N \frac{1}{r_{N+1,i}} = \sum_{\lambda} (U^{(\lambda)} \cdot C^{(\lambda)})$$

(See Racah II, for example).

We then have to work out the products:

$$(\alpha S M_S L \frac{1}{2} m_s l_1 L^T M_L^T | (U^{(\lambda)} \cdot C^{(\lambda)}) | \alpha' S M_S L' \frac{1}{2} m_s l'_1 L'^T M_L'^T).$$

By following the same reasoning as Racah, we obtain the following formula for this expression:

$$\begin{aligned} & (\alpha S M_S L \frac{1}{2} m_s l_1 L^T M_L^T | (U^{(\lambda)} \cdot C^{(\lambda)}) | \alpha' S M_S L' \frac{1}{2} m_s l'_1 L'^T M_L'^T) \\ &= \delta(L^T, L'^T) \delta(M_L^T, M_L'^T) (-)^{L+L'+L^T} W(L_1 L' L_1^T L^T \lambda) \\ & \alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L' \times (\frac{1}{2} m_s l_1 \| C^{(\lambda)} \| \frac{1}{2} m_s l'_1) \quad (69) \end{aligned}$$

These are the reduced elements of the matrix (see Racah II). In the matrix element $(\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L')$ the scalar product affects all atomic variables. We shall then notice this element:

$$((\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L')).$$

As for $(\frac{1}{2} m_s l_1 \| C^{(\lambda)} \| \frac{1}{2} m_s l'_1)$, we see right away that it equals $(l_1 \| C^{(\lambda)} \| l'_1)$.

We can find in the Messiah book the properties of the W coefficients of Wigner. $U^{(\lambda)}$ do not depend upon spins, the element $((\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L'))$ will be nonvariant due to rotation in relation to spins, thus it will not be dependent upon M_S . This fact permits us to make a summation of the Clebsch-Gordan coefficients:

$$\sum_{M_S m_s} \langle S \frac{1}{2} S^T M_S^T | S \frac{1}{2} M_S m_s \rangle \langle S \frac{1}{2} M_S m_s | S \frac{1}{2} S^T M_S^T \rangle = 1. \quad (70)$$

We have. for $V_{\Gamma\Gamma'}(r_{N+1})$:

$$\begin{aligned}
 & V_{\Gamma\Gamma'}(r_{N+1}) \\
 &= \sum_{\lambda} (-1)^{L'+L-\lambda} \delta(L^{\Gamma}, L^{\Gamma'}) \delta(S^{\Gamma}, S^{\Gamma'}) \delta(M_L^{\Gamma}, M_L^{\Gamma'}) \delta(M_S^{\Gamma}, M_S^{\Gamma'}) \\
 & \times (l_1 \| C^{(\lambda)} \| l_1') \cdot W(l_1 L l_1' L', L^{\Gamma} \lambda) ((\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L'))
 \end{aligned}
 \tag{71}$$

where:

$$U_{\mu}^{(\lambda)} = \sum_{i=1}^N U_{\mu}^{(\lambda)}(\hat{t}_i, i, r_{N+1}).$$

Computing Reduced Matrix Elements. -- At present, we have not yet made any supposition on the transition deemed possible and, consequently, it is valid, irrespective of the $\Gamma \neq \Gamma'$ value. (Let us note here that whatever this transition may be, $|L - L'| \leq \lambda \leq L + L'$ according to the very definition of these elements.)

In order to have the $V_{\Gamma\Gamma'}$ potentials correspond to certain given transitions it is sufficient to calculate the reduced element of the matrix:

$$T = ((\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L')). \tag{72}$$

We shall do so for the transition recorded at the start of the chapter:

$$\begin{aligned}
 & (l'^{n-p}(\tau_1 S_1 L_1) l^p(\tau_2 S_2 L_2)) (LS) \\
 & \rightarrow (l'^{n-p-1}(\tau_1' S_1' L_1') l^{p+1}(\tau_2' S_2' L_2')) (L'S').
 \end{aligned}$$

Let us first present the projection of the angular moment of the atom (in accordance with Racah II, formula(29).)

$$\begin{aligned}
 & ((\alpha S M_S L \| U^{(\lambda)} \| \alpha' S M_S L')) = \frac{(-)^{L+M_L}}{V(LL'\lambda - M_L M_L' Q)} \\
 & \times ((l'^{n-p}(\tau_1 S_1 L_1) l^p(\tau_2 S_2 L_2) S L M_S M_L \| U_Q^{(\lambda)} \| \\
 & l'^{n-p-1}(\tau_1' S_1' L_1') l^{p+1}(\tau_2' S_2' L_2'), S L' M_S M_L'))
 \end{aligned}
 \tag{73}$$

The M_L , M_L' and Q are selected in such a manner that:

$$V(LL'\lambda - M_L M_L' Q)$$

be different from zero.

This will give us, according to Racah III (28):

$$\begin{aligned}
 T = & (-)^{L+M_L} [(n-p)(p+1)]^{1/2} \sum_{S_1 L_1} (l'^{n-p} \tau_1 S_1 L_1) \\
 & \left\| \begin{matrix} S_1 L_1 \\ l'^{n-p-1} (\tau_1' S_1' L_1') l' S_1 L_1 \end{matrix} \right\| \\
 & \times [V(LL'\lambda - M_L M_L' Q)]^{-1} \\
 & (l, l^p (\tau_1 S_1 L_1), S_1 L_1' \left\| \begin{matrix} l^{p+1} (\tau_2' S_2' L_2') \\ S_1' L_1' (S_2 L_2), S_2 L_2, SL' \left\| S_1' L_1' l S_2 L_2 (S_2' L_2') SL' \right\| \\ \times (S_1' L_1' l_{n-p} (S_1 L_1), S_2 L_2, SLM_S M_L \\ \times U_Q^{(\lambda)} [n-p, n-p, r_{N+1}] \left\| S_1' L_1' l_{n-p} (S_1 L_1), S_2 L_2, SL' M_S M_L' \right\| \right. \\
 & \quad \quad \quad (74)
 \end{aligned}$$

The coefficients $(l^{n-1} (\alpha_1 L_1 S_1) || S || l^n \alpha LS)$ are fractional parentage coefficients and make possible the separation of one given electron from a group of equivalent electrons. As for the Racah coefficient:

$$(J_1 J_2 (J_3), J_4, J \left\| J_1, J_2 J_4 (J_5), J)$$

they make possible the passing of wave functions obtained in coupling J_1 and J_2 with those obtained by coupling J_1 with the result of the J_2 and J_4 coupling. The expressions for these coefficients are given by Racah (II) and they are quite simply bound to the W coefficients (in the case of an LS coupling). U^λ does not depend upon the spins and we obtain immediately:

$$S_1 = S_3$$

and, in accordance with Racah II (29), T becomes:

$$\begin{aligned}
 T = & [(n-p)(p+1)]^{1/2} \sum_{L_1} (l'^{n-p} \tau_1 S_1 L_1) \\
 & \left\| \begin{matrix} l'^{n-p-1} (\tau_1' S_1' L_1') l' S_1 L_1 \\ (l, l^p (\tau_2 S_2 L_2), S_2 L_2' \left\| \begin{matrix} l^{p+1} (\tau_2' S_2' L_2') \\ S_1' L_1' (S_2 L_2), S_2 L_2, SL' \left\| S_1' L_1' l S_2 L_2 (S_2' L_2') SL' \right\| \\ \times (S_1' L_1' l_{n-p} (S_1 L_1), S_2 L_2, SLM_S M_L \\ \times U^{(\lambda)} (n-p) \left\| S_1' L_1' l_{n-p} (S_1 L_1), S_2 L_2, SL' M_S \right\| \right. \end{matrix} \right. \\
 & \quad \quad \quad (75)
 \end{aligned}$$

We can suppress, in the last reduced element of the matrix the quantum numbers related to the spin. Actually, $U^\lambda(n-p)$ do not depend on the spins and the three groups of electrons which intervene from the left and the right in the scalar product have the same spins, meaning $S_1 = \frac{1}{2}$ and S_2 and the total spin being the same, we can, by revealing the wave functions of the three groups, demonstrate that the reduced matrix element is equal to

$$((L'_1, l'_{n-p}(L_1), L_2, L \| U^\lambda(n-p) \| L'_1 l'_{n-p}(L_3), L_2, L'))$$

Then, by successively applying (44a) and (44b) of Racah III:

$$\begin{aligned} & ((L'_1, l'_{n-p}(L_1), L_2, L \| U^\lambda(n-p) \| L'_1 l'_{n-p}(L_3), L_2, L')) \\ &= (-)^{L_1+L'_1-L'-L} W(L_1 L L_3 L L_2 \lambda) W(l' L_1 L L_3, L'_1 \lambda) \\ & \times [(2L_1+1)(2L_3+1)(2L+1)(2L'+1)]^{1/2} (l' \| U^\lambda \| l). \end{aligned} \quad (76)$$

It remains for us to evaluate $(l' \| U^\lambda(n-p) \| l)$:

$$U^\lambda_\mu = \gamma_\lambda(r_{n-p, n+1}) \widehat{C^\lambda_\mu(n-p)}.$$

The wave functions of the electrons are, respectively:

$$\begin{aligned} \Phi(lm_l) &= \frac{P_{nl}(r_{n-p})}{r_{n-p}} Y^{m_l}_{l'}(\widehat{r_{n-p}}) \\ \Phi(l'm_l) &= \frac{P_{n'l'}(r_{n-p})}{r} Y^{m_l}_{l'}(\widehat{r_{n-p}}) \end{aligned}$$

(the spins having been suppressed a little above.)

Consequently:

$$\begin{aligned} & (l' \| U^\lambda(n-p) \| l) \\ &= \int_0^\infty P_{nl}(r) \gamma_\lambda(r, r_{n+1}) P_{n'l'}(r) dr \times (l' \| C^\lambda \| l) \\ &= \gamma_\lambda(r_{n+1}) \cdot (l' \| C^\lambda \| l) \end{aligned} \quad (77)$$

$(l' \| C^\lambda \| l)$ is a classical quantity equal to:

$$(-)^{l'} [(2l+1)(2l'+1)]^{1/2} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix} \quad \text{ou} \quad \begin{pmatrix} \alpha & \beta & \gamma \\ 0 & 0 & 0 \end{pmatrix}$$

is a symbol $3J$ of Wigner.

Utilizing the expression of the coefficients of Racah given in the book of Messiah, we put T in the form:

$$\begin{aligned}
 T = & [(n-p)(p+1)]^{1/2} (l'^{n-p} \tau_1 S_1 L_1 \{ | l'^{n-p-1} (\tau'_1 S'_1 L'_1) l S_1 L_1 \} (l' \| C^\lambda \| l) \\
 & \times (l, l^p (\tau_2 S_2 L_2)_1 S'_2 L'_2 \{ | l^{p+1} \tau'_2 S'_2 L'_2 \} \cdot [(2S_1+1)(2S'_2+1)(2L+1)(2L'_2+1)(2L_1+1)(2L'+1)]^{1/2} \\
 & \times (-)^{L_1-L+L'_1-L'} W(S_1 \frac{1}{2} S S_2 S_1 S'_2) Y_\lambda(r_{N+1}) \sum_{L_3} (2L_3+1) W(L_1 L L_3 L'_2 \lambda) \\
 & \times W(L'_1 l L'_2 L_3 L'_2) W(l' L_1 l L_3 L'_1 \lambda)
 \end{aligned} \tag{78}$$

Using the symmetrical properties of the W , we can put the last sum over L_3 in the form:

$$(-)^{L_1-L+L'_1-L'} \sum_{L_3} (2L_3+1) W(L'_1 l L L_2 L'_2 L_3) W(L_1 L_2 \lambda L'_1 L L_3) W(\lambda L_1 L'_1 L'_2 L_3)$$

which is, possibly excepting a phase factor, equal to the symbol $9J$ of Wigner $X(abc, def, ghi)$.

Thus, finally for T :

$$\begin{aligned}
 T = & [(n-p)(p+1)]^{1/2} (l'^{n-p} \tau_1 S_1 L_1 \{ | l'^{n-p-1} (\tau'_1 S'_1 L'_1) l S_1 L_1 \} \\
 & \times (l, l^p (\tau_2 S_2 L_2)_1 S'_2 L'_2 \{ | l^{p+1} \tau'_2 S'_2 L'_2 \} (l' \| C^\lambda \| l) W(S_1 \frac{1}{2} S S_2 S_1 S'_2) \\
 & \times [(2S_1+1)(2S'_2+1)(2L+1)(2L'_2+1)(2L_1+1)(2L'+1)]^{1/2} \\
 & \times X(L'_1 L_1 l', L' L \lambda, L'_2 L_2 l) Y_\lambda(r_{N+1})
 \end{aligned} \tag{79}$$

Taking this expression into that of the $V_{rr'}$, we will reach the desired potential.

Starting with this expression for the potential we may see right away what are the λ which will intervene effectively. In the expression of $(l' \| C^\lambda \| l)$ there is the symbol $3J \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}$ which equals zero except in cases where $l+l'+\lambda$ is an even number, which immediately

determines the parity of λ . In addition, in order to avoid the $\begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}$ being a zero it is necessary to have the three numbers l , λ and l' verifying the triangular inequalities, from where $|l - l'| \leq \lambda \leq l + l'$. The same applies to $W(l_1 L_1', L_1' L_1 \lambda)$ which will not be a zero only in the case where the six factors verify, three to three, the triangular inequalities (14).

The $V_{\Gamma\Gamma'}$ Expressions for Certain General Transitions.

Transition 1 :

$$\begin{aligned}
 & l^n(\alpha LS) \rightarrow l^n(\alpha' L' S') \quad (\alpha LS) \neq (\alpha' L' S') \\
 V_{\Gamma\Gamma'}(r_{N+1}) = & \sum_{\alpha, L_1 S_1 \lambda} (-)^{L_1 + \lambda - L_1' + L + L'} \delta(L^\tau, L^{\tau'}) \delta(S^\tau, S^{\tau'}) \delta(M_L^\tau, M_L^{\tau'}) \delta(S_1 S_1') \delta(M_s^\tau, M_s^{\tau'}) \\
 & \times \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix} (2l+1) [(2L+1)(2L'+1)(2l_1+1)(2l_1'+1)]^{1/2} \cdot W(l L L_1' L_1 \lambda) \quad (80) \\
 & \times W(l_1 L_1' L_1' L^\tau \lambda) \cdot n(l^n \alpha LS \mid \mid l^{n-1}(\alpha_1 S_1 L_1) LS) (l^{n-1}(\alpha_1 L_1 S_1) SL' \mid \mid l^n \alpha' L' S) \\
 & \times Y_\lambda(r_{N+1})
 \end{aligned}$$

Transition 2 :

$$\begin{aligned}
 & \{ l_2^m(\tau_1 S_1 L_1) l^n(\alpha S_1 L_1) \} \mid LS \mid \rightarrow \{ l_2^m(\tau_1 S_1 L_1) l^n(\alpha' S_1' L_1') \} \mid L' S' \mid \quad (\alpha L_1) \neq (\alpha' L_1') \\
 V_{\Gamma\Gamma'}(r_{N+1}) = & \sum_{\alpha, L_1 S_1 \lambda} (-)^{L_1 + \lambda - L_1' + L + L'} \delta(L^\tau, L^{\tau'}) \delta(S^\tau, S^{\tau'}) \delta(M_s^\tau M_s^{\tau'}) \delta(M_L^\tau M_L^{\tau'}) \\
 & \times \delta(SS') \delta(S_1 S_1') \begin{pmatrix} l & l & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix} [(2l_1+1)(2l_1'+1)(2L_1+1)(2L_1'+1)(2L+1)(2L'+1)]^{1/2} \quad (81) \\
 & \times (2l+1) \cdot n \cdot W(l L_1 L_1' L_2 \lambda) W(l_1 L_1' L_1' L^\tau \lambda) W(L_2 L' L_1 \lambda L_1' L) \\
 & \times (l^n \alpha S_1 L_1 \mid \mid l^{n-1}(\alpha_1 S_2 L_2) L S_1 L_1) (l^{n-1}(\alpha_1 S_2 L_2) L S_1 L_1' \mid \mid l^n \alpha' S_1' L_1') Y_\lambda(r_{N+1})
 \end{aligned}$$

Transition 3 :

$$\begin{aligned}
 & \{ l^{n-p}(\tau_1 S_1 L_1) l^p(\tau_2 S_2 L_2) \} \mid LS \mid \rightarrow \{ l^{n-p-1}(\tau_1' S_1' L_1') l^{p+1}(\tau_2' S_2' L_2') \} \mid L' S' \mid \\
 V_{\Gamma\Gamma'}(r_{N+1}) = & \sum_{\lambda} (-)^{L - L' + 1} \delta(L^\tau, L^{\tau'}) \delta(S^\tau, S^{\tau'}) \delta(SS') \delta(M_L^\tau, M_L^{\tau'}) \delta(M_s^\tau, M_s^{\tau'}) \\
 & \times [(n-p)(p+1)]^{1/2} \cdot (l^{n-p}(\tau_1 S_1 L_1) \mid \mid l^{n-p-1}(\tau_1' S_1' L_1') l^p S_1 L_1) (l, l^p(\tau_2 S_2 L_2), S_2' L_2' \mid \mid l^{p+1}(\tau_2' S_2' L_2')) \\
 & \times \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix} W(S_1' \frac{1}{2} S S_2 S_2') W(l_1 L_1' L_1' L^\tau \lambda) \cdot X(L_1' L_1 l' L' L \lambda L_2' L_2 \lambda) \quad (82) \\
 & \times [(2S_1+1)(2S_2+1)(2l+1)(2l'+1)(2L_2+1)(2L_1+1)(2L+1)(2L'+1)(2l_1+1)(2l_1'+1)]^{1/2} \\
 & \times Y_\lambda(r_{N+1})
 \end{aligned}$$

Transition 4 :

$$\begin{aligned}
 & \{ l_2^m(\tau_2 S_2 L_2) l^n(\tau_1 S_1 L_1) \} \{ LS \} \rightarrow \{ l_2^m(\tau_2 S_2 L_2) (l^{n-1}(\tau_4 S_4 L_4) l') (S_1' L_1') \} \{ LS' \} \\
 V_{\Gamma\Gamma'}(r_{N+1}) = & \sum_{\lambda} (-)^{l'+L_1-L'+L_1} [n(2L+1)(2L'+1)(2L_1+1)(2L_1'+1)(2l+1)(2l'+1) \\
 & \times (2l_1+1)(2l_1'+1)]^{\frac{1}{2}} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix} W(l_1 l' L_1' L_4 \lambda) W(L_2 L' L_1 \lambda L_1' L) \\
 & \times \begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix} W(l_1 L_1' L' L \lambda) \cdot (l^n(\tau_1 S_1 L_1) \{ l^{n-1}(\tau_4 S_4 L_4) l S_1 L_1 \} \\
 & \times Y_{\lambda}(r_{N+1}) \delta(S^r, S'^r) \delta(L^r, L'^r) \delta(SS') \delta(M_a^r, M_s^r) \delta(M_L^r, M_L'^r)
 \end{aligned} \quad (83)$$

We notice that $\begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}$ require zero or even λ for transition 1 and 2.

In the case where $L + L' + \lambda$ is even, we can avoid a certain part of the work by utilizing the coefficients which were listed in tables by Percival and Seaton (13) and which have the great advantage of being easily computable. These coefficients have the following form:

$$f_{\lambda}(l_1 L_1' L' L \lambda) = [(2l_1+1)(2l_1'+1)(2L+1)(2L'+1)]^{\frac{1}{2}} \begin{pmatrix} l_1 & l_1' & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & L' & \lambda \\ 0 & 0 & 0 \end{pmatrix} (-)^{L+L'-L} W(l_1 L_1' L' L \lambda) \quad (84)$$

equivalent to that of formula (53).

III. Applying Resonance Radiation to Excitation in the Isoelectronic Series of Lithium and Sodium

We have used the Coulomb-Born method to calculate the terms of the R matrix, the method called CB II, where the terms of the T matrix are given by the exact equation (40) as opposed to CB I in which the T is given by the equation (39). As a matter of fact, in order to achieve intense transitions in positive ions, it is necessary to take into account the Coulomb field which appears due to the residual charge of the ion, and, on the other hand, to consider the effects of strong couplings.

Solving a collision problem involves, first of all, a knowledge of the amplitude probabilities of the atomic electron. We have used, for the 2s and 2p states of the lithium series analytical wave functions of the hydrogenide order (24). The use of these simple forms for the above series is justified providing it is apparent that the quantum errors are small and the calculations of probabilities of radiative transitions attain by and large the same results, whether the Hartree Fock functions or the hydrogenide functions are used as it is done, for instance, by Bates and Damgaard (3). For $2s \rightarrow 2p$ in lithium we find 0.75 for the oscillating force when using the latter method, which is precisely the result of the experiment.

For the states 3s and 3p of the sodium series we have used the same wave functions as we used for Mg II, Si IV and Fe XVI. For Mg II these functions have been computed by Biermann and Lubeck (6) in a Thomas Fermi field, taking into account the exchange potential and the polarization. The wave functions for Si IV have been calculated by the Hartree Fock method (11). The more recent calculations of Garstang (10) which take into account polarization effects do not modify, to any significant extent, the preceding results. We have used for Fe XVI the wave functions of Hartree Fock which were kindly passed on to us by Dr. S.J. Czyzak.

Besides, in principle, in the development (4) of the total wave function of the system all bound states and the continuum of the atom must intervene. We have reduced the atom to two levels, 2s and 2p for

the lithium series and to 3s and 3p for the sodium series. We have mentioned above the meaning of this approximation. Only intense transitions generated from the p and s levels can affect the cross-section corresponding to the transition $s \rightarrow p$. Let us consider the case of the sodium series. If -- as is the case, -- the resonance transition $3s \rightarrow 3p$ is optically intense (F is large) in accordance with the Thomas Kuhn law, the other transitions $3s - np$ will be weak. We find that the most intense transition generated from 3p is $3p \rightarrow 3d$. Thus it is extremely important to take into account the level 3d; this has been done in another case, involving the case of Ca II (20) for which we have demonstrated that disregarding the 3d level is tantamount to overestimation of the cross-section $4s \rightarrow 4p$ of 25 p. 100. In the Li and Na series, however, contrary to what occurs in Ca II, the energy of the 3d level above the ground level is of the order of three times the excitation energy of the 3p level (or 2p in the case of Li). It is quite possible to show that in this case the error made by disregarding the couplings with 3d is considerably smaller than 25 p. 100; as a matter of fact, the terms of the R matrix diminish with the energy difference $E_d - E_p$.

Calculating the Terms of the R Matrix

When the total kinetic moment L^T is conserved, the elements of the R_{ij} matrix which correspond to two different L^T , will be zero. Consequently, the total R matrix (which is infinite) is placed in the form of an infinite Jordan matrix, in other words as square matrices on the

diagonal. Each of these matrices corresponds to a value L^T . For all practical purposes only a definite number of values of L^T could make a contribution to the total cross-section Q , as the elements of the R_{ij} matrix rapidly decrease with the L^T . We will see that depending upon the energy of primary electrons we will have to take into account 10 to 15 values of the kinetic moment.

With two atomic levels s and p what will be the dimension of each $R(L^T)$ matrix corresponding to the value of the kinetic moment? By applying the coupled presentation as in formula (45) to a level s ($L = 0$) we can associate only the kinetic moment $l=L^T$ in order to obtain L^T . At the level p we may associate the kinetic moments to the primary electron:

$$l = L^T - 1, \quad l = L^T, \quad l = L^T + 1$$

in order to obtain L^T . The matrices will thus be of dimension 4. Except for the case of $L^T = 0$ where only $L^T + 1$ can be associated to p in order to obtain L^T . In the case of $L^T = 0$ the matrices will be of the 2 order. The states of the system will be characterized by quantum numbers:

$$\begin{aligned} \Gamma_1 &= (n_s, s, L^T, L^T) & \Gamma_2 &= (n_p, p, L^T - 1, L^T) \\ \Gamma_3 &= (n_p, p, L^T, L^T) & \Gamma_4 &= (n_p, p, L^T + 1, L^T). \end{aligned}$$

The elements of the R matrix are calculated starting from the equations (29) and (45). After having explicitated the slope coefficients and in considering the equations (46):

$$\begin{aligned} R_{11} &= -2\mathcal{R}_0(sL^T, sL^T) \\ R_{22} &= -2[\mathcal{R}_0(pL^T - 1, pL^T - 1) \\ &\quad + 0,2(L^T - 1)[2L^T - 1]^{-1/2}\mathcal{R}_2(pL^T - 1, pL^T - 1)] \\ R_{33} &= -2[\mathcal{R}_0(pL^T, pL^T) + 0,2\mathcal{R}_2(pL^T, pL^T)] \\ R_{44} &= -2[\mathcal{R}_0(pL^T + 1, pL^T + 1) \\ &\quad + 0,2(L^T + 2)[2L^T + 1]^{1/2}\mathcal{R}_2(pL^T + 1, pL^T + 1)] \\ R_{12} &= -2\left[\left(\frac{L^T}{6L^T + 3}\right)^{1/2}\mathcal{R}_1(sL^T, pL^T - 1)\right] \end{aligned}$$

$$\begin{aligned}
R_{14} &= -2 \left[- \left(\frac{L^r + 1}{6L^r + 3} \right)^{\frac{1}{2}} \mathcal{R}_1(sL^r, pL^r + 1) \right] \\
R_{24} &= -2 \left[- \frac{0,6}{2L^r + 1} (L^r(L^r + 1))^{\frac{1}{2}} \mathcal{R}_2(pL^r - 1, pL^r + 1) \right] \\
R_{13} &= 0 \quad R_{23} = 0 \quad R_{34} = 0.
\end{aligned}
\tag{31}$$

In calculating the terms of the R matrix, as in the equations (41) and (45) we neglected the short-range terms which are due to the closed shells.

We will note that R_{33} is uncoupled and that, consequently, it will intervene only in calculations relating to the $p \rightarrow p$ transitions. On the other hand, the diagonal terms and the terms R_{24} , the elastic terms, rapidly become very small for $L^r > 2$ as compared to the inelastic terms R_{14} and R_{13} . This is quite fortunate as their calculation by approximation as devised by Born brings very unsatisfactory results. We can demonstrate, in fact, that radial terms \bar{R}_0 and \mathcal{R}_2 are "short-range" terms which essentially cause the intervention of small values of the variable radial r , meaning of areas where it is impossible to state whether the collision electron is placed in a Coulomb field. If diagonal terms are to be taken into account and correctly calculated it is necessary to solve the system of coupled equations (13). One of us performed this task (5) and arrived at the following result: the solution of coupled equations actually shows only 10 p. 100 difference with results obtained for the inelastic cross-section $s \rightarrow p$ of Be II with low energy, as shown by results obtained by using the CB II method, used here disregarding the elastic terms (See fig. 4).

The cross-section $Q(nL \rightarrow n'L')$ given by the equation (59) will bring about the intervention only of the T_{12} and T_{14} inelastic elements. We have now demonstrated that the influence of small R_{ij} elastic terms was small. The R matrix which we shall calculate will have the simple

form:

$$R^{en} = \begin{vmatrix} 0 & R_{12} & R_{14} \\ R_{12} & 0 & 0 \\ R_{14} & 0 & 0 \end{vmatrix} \quad (86)$$

In applying formula (40) to the CB II approximation:

$$T_{12} = \frac{-2iR_{12}}{1 + R_{12}^2 + R_{14}^2} \quad T_{14} = \frac{-2iR_{14}}{1 + R_{12}^2 + R_{14}^2} \quad (87)$$

In the CB I approximation equivalent to the Born approximation:

$$R_{12} = -2iR_{12} \quad T_{14} = -2iR_{14} \quad (88)$$

The cross-section will be expressed as:

$$Q[nL=0, n'L'=1] = \frac{1}{k_{nL}^2} \frac{1}{2L+1} \sum_{L^r} (2L^r+1) [T_{14}^2(L^r \rightarrow L^r+1) + T_{12}^2(L^r \rightarrow L^r-1)] \quad (89)$$

All calculations relative to the radial terms R_λ whose expressions have been presented above have been built according to the methods explained by one of our group (20) by means of ordinator 650 and 704 IBM.

Results

Results for transitions $2s - 2p$ of the four elements of the Li series and for transitions $3s - 3p$ of three elements of the Na series are presented in tables I and II. It is thus possible to obtain by interpolation the cross-section of any desired element in each series.

Table I Lithium series $\Omega(\text{CB I})$ et $\Omega(\text{CB II})$.

X	Be II		C IV		O VI		Mg X	
	CB I	CB II	CB I	CB II	CB I	CB II	CB I	CB II
1	14,23	9,983	5,015	4,669	2,526	2,456	1,208	1,200
2	16,73	13,44	5,588	5,304	2,812	2,754	1,318	1,307
3	17,80	15,03	5,940	5,694	2,963	2,911	1,372	1,360
4	18,38	16,04	6,133	5,915	3,047	3,000	1,404	1,395
5	18,96	16,95	6,269	6,074	3,180	3,137	1,433	1,424
6	19,58	17,73	6,438	6,261	3,312	3,271	1,450	1,440

Table II

Sodium Series

X	Mg II		S IV		Fe XVI	
	CB I	CB II	CB I	CB II	CB I	CB II
1	17,69	11,74	10,47	9,351	1,712	1,696
1,5	19,89	14,60	11,12	9,958	1,756	1,742
2	21,75	16,98	11,73	10,66	1,800	1,781
4	27,41	24,02	13,65	12,88	1,952	1,939

In these tables we present the probability values $\Omega(s \rightarrow p)$ bound to the cross-sections by the relation (60).

$$Q(nL \rightarrow n'L') = \frac{1}{2L+1} \frac{1}{k_{nl}^2} \Omega(nL, n'L'), \quad (89)$$

in units of πa_0^2

k_{nL}^2 is the initial kinetic energy in Ryndbergs.

The results are presented as a function of the relation of the initial kinetic energy and the energy difference $E_{n'L'} \rightarrow E_{nL}$:

$$X = \frac{k_{nl}^2}{(E_{n'L'} - E_{nl}) \text{ Rydbergs}} \quad (90)$$

It should be noted while studying tables I and II that in the high energy areas there is but a small difference between the CB II approximation and the CB I approximation, which is equivalent to the Born approximation for neutrals.

On the other hand, as we become involved with elements more strongly ionized, the CB I approximation becomes better and sometimes even sufficient, even at the excitation threshold ($X = 1$). In fact, the influence of the $V_{rr'}$ coupling terms in coupled equations (13) becomes secondary when the residual charge of the positive ion increases to a large extent.

The cross-section values are presented in figures 1 and 2. Inasmuch as these vary greatly as Z^{-4} (which would be the case of purely hydrogenoid ions), but more precisely as the square of the relation of excitation energies, we have transformed the results in order to be able to trace them on one chart.

It should be noted that in Figure 2 the curve relative to Mg II does not run above the two other curves as could have been expected. The results presented in these figures are those obtained using the CB II approximation; yet it is immediately apparent from looking at Table II that in the case of Mg II the effects of coupling (CB II - CB I) are particularly important. The resonance transition $3s - 3p$ of Mg II is highly intense ($f = 0.90$), thus, similarly, the elements of the matrices R_{12} and R_{14} , as we shall see later on; this fact explains the important difference between the approximations (87) and (88).

The dipolar terms of the R matrix vary as $1/\Delta E_{nL}$, thus they decrease as Z^{-2} in the first approximation. The coupling effects thus become rapidly negligible when Z increases.

It would seem to be of interest to present certain results in relation to the contributions to different kinetic moments L^T . We present the values of the $\Omega_{L,T}$ for Mg II and Fe XVI in Figure 3. We have:

$$\Omega[nL, n'L'] = \sum_{L,T} \Omega_{L,T}(nL, n'L'). \quad (91)$$

We can see that the contributions of small kinetic moments diminish when the electron energy increases and also when the residual charge increases. This contribution is always small and this is sufficient to

justify the use of the method applied by us. This method is in fact deficient for the small values of L^T which correspond to the "approximated" collisions for which the exchange effects and the exact form of the potential close to the nucleus are very important. As stated above, we have also disregarded in the calculations of the matrix R the elastic terms, but the latter intervene in a significant manner only in the cases of $L_T = 0$ or 1.

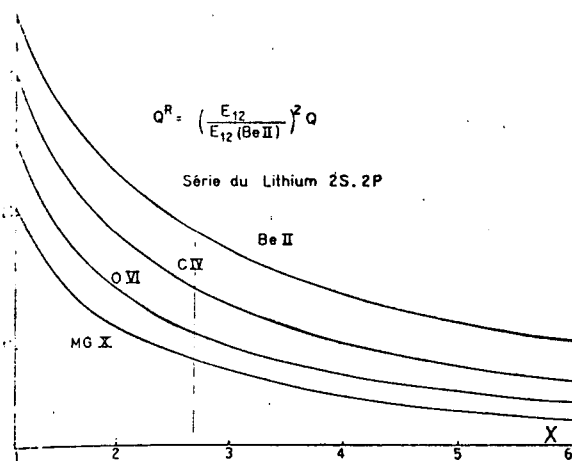


FIG. 1.

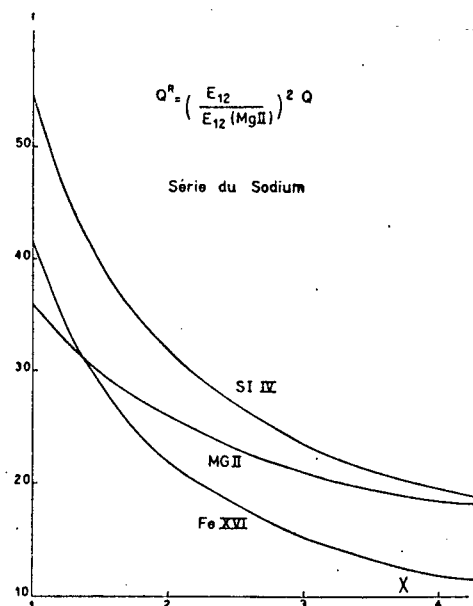


FIG. 2.

Consequently, if only a very limited confidence should be extended to the results of Ω_L^T for $L_T = 0$ or 1, the error made in this manner will affect in a very insignificant way the global result Ω . The calculations in relation to the positive ions are, thus, much more reliable than those in relation to neutral atoms, for which the small

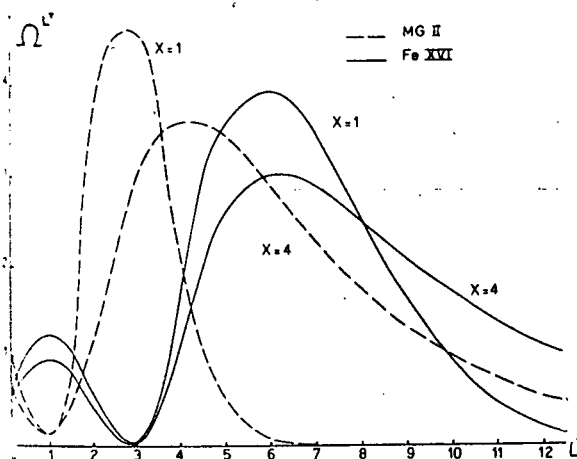


FIG. 3.

values of L^T which correspond to the "approximated" collisions for which the exchange effects and the exact form of the potential close to the nucleus are very important. As stated above, we have also disregarded in the calculation of the matrix R the elastic terms, but the latter intervene in a significant manner only in the cases of $L_T = 0$ and 1 .

Consequently, if only a very limited confidence should be extended to the results of Ω_L^T for $L_T = 0$ or 1 , the error made in this manner will affect in a very insignificant way the global result Ω . The calculations in relation to the positive ions are, thus, much more reliable than those in relation to neutral atoms, for which the small values of L^T are more important at low energies.

If we look for partial sections, which would correspond to the transitions between two definite levels by quantum numbers $nLSJ$ where \vec{S} is the spin and $\vec{J} = \vec{L} + \vec{S}$ the total angular momentum, we will notice that the total system will be either a singlet or a triplet:

$$\begin{aligned}
 & (S^T = 1, S^T = 0) \\
 \Omega(nLS, n'L'S') &= \frac{1}{2} \sum_{s^T L^T} (2L^T + 1)(2S^T + 1) |T|^2 \\
 &= 2\Omega(nL, n'L')
 \end{aligned} \quad (92)$$

because T is independent from S^T when the exchange and the spin-orbit are disregarded.

Consequently, inasmuch as $S = \frac{1}{2}$ in relation to the initial s level:

$$Q[nLS \rightarrow n'L'S'] = Q[nL \rightarrow n'L']. \quad (93)$$

On the other hand, if there is the case of an LS coupling we can demonstrate that for a transition coming from the s level:

$$\begin{aligned}
 & Q[nLSJ \rightarrow n'L'S'J'] \\
 &= \frac{2J' + 1}{(2S' + 1)(2L' + 1)} Q[nLS \rightarrow n'L'S']. \quad (94)
 \end{aligned}$$

In other words, the partial sections are in relation to the statistical weights:

$$\begin{aligned}
 Q\left[s \frac{1}{2} \rightarrow p \frac{1}{2}\right] &= \frac{1}{3} Q[s \rightarrow p] \\
 Q\left[s \frac{1}{2} \rightarrow p \frac{3}{2}\right] &= \frac{2}{3} Q[s \rightarrow p].
 \end{aligned} \quad (95)$$

The Bethe Approximation in the Case of Positive Ions

The Bethe approximation is generally considered as a simplification of the Born approximation, quite valid in the case of high energies when the deflection $\vec{K} = \vec{k}_i - \vec{k}_j$ is small in relation to the initial impulse \vec{k}_i of primary electrons.

We can find the Bethe approximation by a process which is quite different and valid for neutral atoms as well as for positive ions (21). It is sufficient to give to the electrostatic interaction term for any value of r_1 and r_2 its form as deduced from (42) when $r_2 > r_1$ which actually means that there is a supposition that the collision electron is still outside the atom:

$$\frac{1}{r_{12}} = \sum_{\lambda} P_{\lambda}(\hat{r}_1, \hat{r}_2) \frac{r_1^{\lambda}}{r_2^{\lambda+1}}. \quad (96)$$

This approximation is in fact valid for the large values of L_T for which the small values of r_2 do almost no intervening.

We shall notice that the calculations of integral radials and of the terms of the R matrix are then considerably simplified. We have, in relation to formula (47):

$$\begin{aligned} & R[nLlL', n'L'l'L'] \\ &= -2f_1(LlL'l'L') \int_0^{\infty} F_n F_{k'} \frac{1}{r^2} dr \int_0^{\infty} P_{nl} P_{n'l'} r dr \quad (97) \end{aligned}$$

for a dipolar transition. The approximation (96) evidently, cannot be applied in the cases of elastic terms or to the $\lambda = 2$ terms of quadrupolar transitions in which the electrostatic interaction near the nucleus (r small, L_T small) plays an important part.

The Bethe approximation, in addition, implies another approximation, that which consists in using (88), meaning the disregard for any effect of strong coupling.

It can be shown that, in this case, the very simple expression of Bethe is regained. Having recognized the elements of the matrices $\int P_{nl} P_{n'l'} r dr$ of the probability of the dipolar radiative transition, we

obtain (21):

$$Q[nL \rightarrow n'L'] = \frac{8\pi}{\sqrt{3}} \frac{1}{k_{nL}^2} \frac{I_H}{E_{n'L'} - E_{nL}} f(n'L', nL) g(k_{nL}, k_{n'L'}) \quad (98)$$

where I_H is the ionization^{energy} of hydrogen.

The oscillator force f is expressed:

$$f(n'L', nL) = \frac{1}{3} \frac{E_{n'L'} - E_{nL}}{I_H} \frac{L_{>}}{2L+1} \left| \int_0^\infty P_{nL} P_{n'L'} r dr \right|^2 \quad (99)$$

where $L_{>}$ is the largest of the numbers L or L' .

The Gaunt factor g is expressed:

$$g(k_{nL}, k_{n'L'}) = \sum_{ll'} \frac{2\sqrt{3}}{\pi} l_{>} \left| \int_0^\infty F_{kl} F_{k'l'} \frac{dr}{r^2} \right|^2 \quad (100)$$

In the case of neutral atoms the collision electron is presented after as well as before the collision by plane waves, the functions of F are the Bessel spherical functions and we regain the well-known form:

$$g(kk') = \frac{\sqrt{3}}{\pi} \log \frac{(k+k')}{(k-k')}. \quad (101)$$

We shall designate the Bethe approximation by CB'I; it consists in utilizing the formula (98). The results are presented in Tables III and IV.

Table III
Lithium Series; Ω values

X	Be II		C IV		O VI		Mg X	
	Bethe I	Bethe II	Bethe I	Bethe II	Bethe I	Bethe II	Bethe I	Bethe II
1	26,52	14,04	7,373	6,649	3,411	3,232	1,265	1,254
2	30,96	18,63	8,224	7,540	3,731	3,620	1,379	1,368
3	33,61	21,13	8,855	8,155	3,989	3,878	1,435	1,425
4	35,51	22,82	9,302	8,580	4,190	3,995	1,476	1,465
5	37,19	24,30	9,652	8,900	4,338	4,224	1,508	1,497
6	38,42	25,32	10,025	9,239	4,487	4,374	1,529	1,512

Table IV
Sodium Series; Ω values

X	Mg II		Si IV		Fe XVI	
	Bethe I	Bethe II	Bethe I	Bethe II	Bethe I	Bethe II
1	45,22	16,98	19,59	15,04	2,172	2,147
1.5	49,25	21,02	20,78	16,32	2,250	2,226
2	52,85	24,46	21,92	17,59	2,329	2,302
4	64,06	34,65	25,81	21,18	2,609	2,583

We can immediately conceive the possibility of performing the first approximation (96) without performing the second (88), which amounts to taking into account --- in spite of anything --- the effects of strong coupling. This second method will be designated by Bethe as CB' II. It will consist of calculating terms due to (97) and to then utilize the precise formula (87). As it is quite easy to calculate the integrals which appear in (97) for which analytical equations exist (20), we gain, in this manner, the possibility of easily obtaining results which prove to be considerably better than could be expected.

The figures 4 and 5 present cross-sections $Q(2s \rightarrow 2p)$ for Be II and for C IV, as we have devised them. We can see that in relation to the most effective approximation (CB II), it is the part played by the coupling in CB' II, in bringing in the most important correction to the Bethe approximation CB' I as in the case of Be II. This phenomenon is more apparent still in Mg II (22) and is dependent on the intensity of resonance transitions in Be II and Mg II.

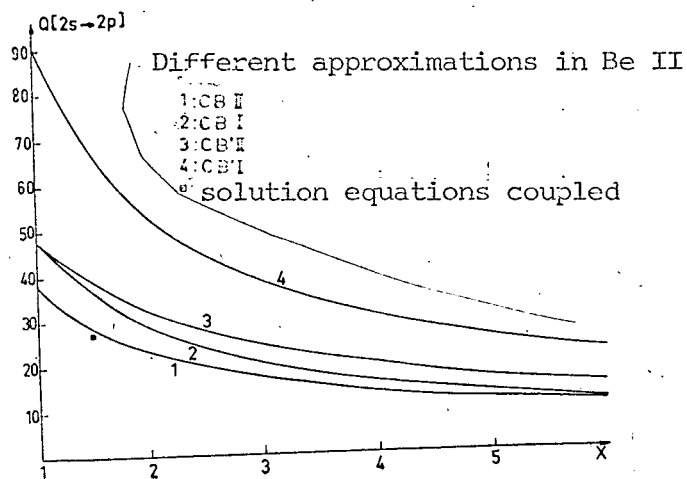


FIG. 4.

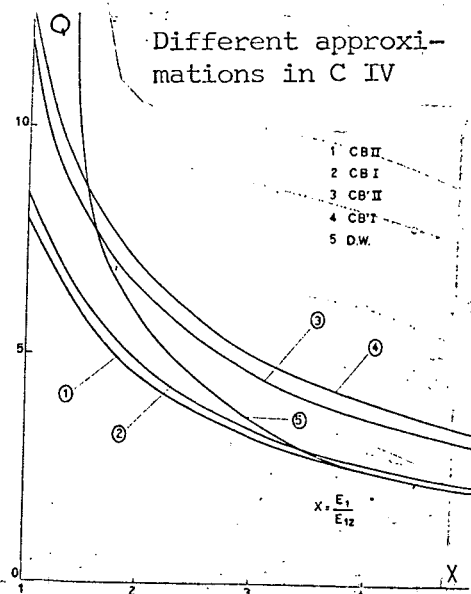


FIG. 5.

When Z increases, on the other hand, the part played by the strong coupling effects diminishes and there remains, between the two approximations (that of Coulomb-Born and that of Bethe), the only difference brought about by the use of (96). This difference itself decreases gradually as we deal with more strongly ionized elements and this is understandable when -- as in Figure 3 -- we perform the decomposition into sub-waves.

It seems suitable to express all these effects in terms of an empirical Gaunt factor \bar{g} defined by the formula:

$$Q = \frac{8\pi}{\sqrt{3}} \frac{1}{k_i^2} \frac{I_{ii}}{E_j - E_i} / (j, i) \bar{g} \quad \text{en } \pi a_0^2 \quad (102)$$

In order to determine the \bar{g} we will calculate Q by the CB II and CB I method. We find for the Na series:

Table V

X	Mg II		Si IV		Fe XVI	
	CB I	CB II	CB I	CB II	CB I	CB II
1,0	0,426	0,282	0,567	0,496	0,816	0,808
1,5	0,479	0,352	0,603	0,540	0,837	0,830
2	0,524	0,409	0,635	0,578	0,858	0,850
4	0,661	0,579	0,740	0,698	0,930	0,924

We find that not very far from the threshold the \bar{g} is of the unit order. This means that when Z increases, the Bethe approximation provides the best results. In several previous articles (16) (23) it has been suggested that, in general, the $\bar{g} = 0.2$ near the excitation threshold. This empiric determination of \bar{g} is the result of reduction of a certain number of measures and calculations made for slightly ionized

elements. It is also in accordance with the results achieved by Burgess (7) for hydrogen ions.

When \bar{g} increases with Z in a much more rapid manner than foreseen by the Burgess results it means that, contrary to the processes in the isoelectronic series of H, the oscillating forces decrease with Z , which diminishes the effects of strong couplings. On the other hand, the effect of the repelling screen of the inner-shell electrons diminishes the probabilities of approximated collisions for which the Bethe (96) approximation is no more valid.

Comparison With Results of the

Semi-Classical Theory

The semi-classical theory, also called the impact parameter theory, is widely used in nuclear physics (1) and in collision problems of heavy particles (2); it has recently been applied by Seaton (17) to the computation of inelastic collisions of neutral atoms and electrons.

A. Burgess has expanded the method to the case of positive ions. In the majority of cases it is possible to obtain a good evaluation of the section radius in the integration over the collision parameter and find, in this manner, precise cross-sections for dipolar transitions, cross-sections with high energies and better results than those achieved by using the Born approximation with low energies:

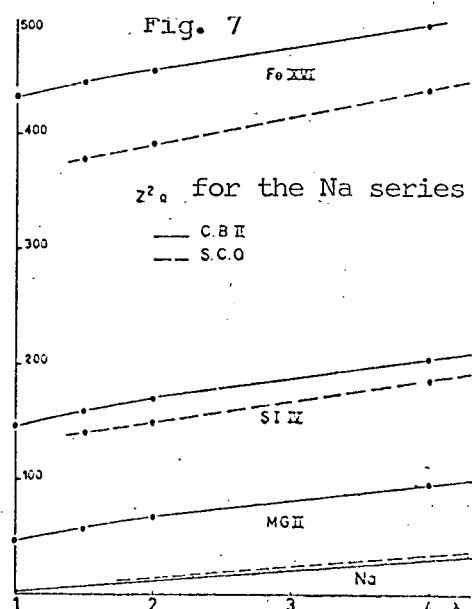
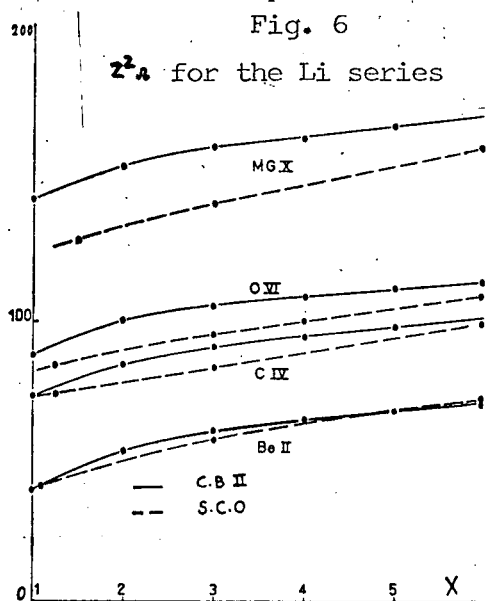
$$Q(i \rightarrow j) = \int_{n_0}^{\infty} P_{ij}(R) 2\pi R dR \quad (103)$$

where the excitation probability $P_{ij}(R)$ depends mainly upon the oscil-

lation force $f(j, i)$ and where R_0 , the section radius can, generally, be considered as being equal to the smallest of the median radii of \bar{r}_i or \bar{r} , becoming \bar{r} .

The comparison of our results (CB II) with those obtained by using the semi-classical method (sco) are presented in figures 6 and 7. We can see that there is a complete agreement as far as the first elements of the series are concerned. The two curves practically coincide in the case of Mg II.

The agreement is satisfactory for the sodium (17). In figure 7, presenting Na the solid line curve is that of experimental results. Starting with the Vainstein calculations (19), Sommerville (18) has demonstrated that using a method only slightly different from the Born II method it is possible to establish $3s \rightarrow 3p$ results only slightly different from experimental results.



For strongly ionized elements the semi-classical approximation becomes less satisfactory. As the Z augments, the $f(ji)$ decreases with

Z while the energy difference ΔE_{ij} increases as Z^2 . Thus the relation tends to become zero. Yet, Seaton (17) has shown that in this case it was not possible any more to take $R_0 = \bar{r}_0$ and that it was necessary to determine R_0 in such a manner as to find the exact cross-sections with high energies.

In any case the difference does not exceed 20 p. 100 and the semi-classical method makes possible to obtain, quite easily, a good evaluation of collision cross-sections. This shows again, that in the excitation of transitions optically permissible, large values of the L^T play a predominant part, the values with which an impact parameter may be made to correspond when the collision electron is displaced along a classic trajectory.

We would like to take this occasion to thank Prof. M.J. Seaton of the University College (London) who has introduced us to the collision theory and we owe to him the existence, in the Meudon Observatory, of a group interested in this chapter of physics, indispensable to the progress of astrophysics as a study of ionized media. We also owe gratitude to the doctors S.J. Czyzak and A. Burgess who gave us permission to use articles not yet published. We will end our article by expressing the wish to have more contact among all those in France who are interested in problems of atomic collisions.

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